

1,3-diphenyl-1,3-diazetidine  
74949-76-1 | DTXSID60321268

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

## Model Results

**Predicted value:** 156 °C

**Global applicability domain:** Inside

**Local applicability domain index:** 6.67e-01

**Confidence level:** 3.89e-01

## Nearest Neighbors from the Training Set

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Clomipramine

**Measured:** 190

**Predicted:** 163

Image not found

Imipramine

**Measured:** 175

**Predicted:** 145

Image not found

Imipramine hydrochloride

**Measured:** 174

**Predicted:** 145

Image not found

Trimipramine

**Measured:** 45.0

**Predicted:** 119

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N,N,N',N'-Tetramethylbenzidine

**Measured:** 194

**Predicted:** 153